

Mott metal-insulator transition in the Hubbard model

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The ground state of the Hubbard model is studied within the single-site approximation (SSA) and beyond the SSA. Within the SSA, the ground state is a typical Mott insulator at the critical point $n = 1$ and $U/W = +\infty$, with n being the electron density per unit cell, W the bandwidth of electrons, and U the on-site repulsion, and is a normal Fermi liquid except for the critical point. Beyond the SSA, the normal Fermi liquid is unstable against a non-normal Fermi liquid state except for a trivial case of $U = 0$ such as a magnetic or superconducting state in two and higher dimensions. In order to explain actual observed metal-insulator transitions, one or several effects among the electron-phonon interaction, multi-band or multi-orbital effects, and effects of disorder should be considered beyond the Hubbard model.

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The Mott metal-insulator (M-I) transition is an interesting and important issue in solid-state physics [1], and a lot of effort has been made towards clarifying it [2]. However, its theoretical treatment is still controversial. One of the most contentious issues is whether or not the transition can be explained within the Hubbard model.

In Hubbard's approximation [3, 4], a band splits into two subbands when the on-site repulsion U is large enough such that $U \gtrsim W$, with W the bandwidth ($W > 0$); the subbands are called the upper Hubbard band (UHB) and the lower Hubbard band (LHB). In Gutzwiller's approximation [5, 6], a narrow quasiparticle band appears around the chemical potential; the band and quasiparticles are called the Gutzwiller band and quasiparticles. It is plausible to speculate that the density of states in fact has a three-peak structure, with the Gutzwiller band between UHB and LHB. Both of the approximations are single-site approximations (SSA). Another SSA theory [7] confirms this speculation, showing that the Gutzwiller band appears at the top of LHB when the electron density per unit cell n is less than one, i.e., $n < 1$. According to Kondo-lattice theory [8, 9, 10], the three-peak structure corresponds to the Kondo peak between two subpeaks in the Anderson model, which is an effective Hamiltonian for the Kondo problem. An insulating state can only be realized when the Fermi surface (FS) of the Gutzwiller quasiparticles vanishes.

When $n = 1$ and $W/U = 0$, a localized electron or a non-interacting spin sits at every unit cell. In this case, the ground state is infinitely degenerate and is a typical Mott insulator. In Gutzwiller's approximation, the ground state is a metal for $n \neq 1$ or $W/U > 0$. According to Brinkman and Rice's theory [11], when $n = 1$ the effective mass of the quasiparticles diverges at a critical $U \simeq W$, which is denoted as U_{BR} here. It may be argued that the FS of the quasiparticles vanishes for $n = 1$ and $0 \leq W/U \leq W/U_{BR}$, i.e., on the dashed line in the phase diagram shown in Fig. 1. It is curious that no order parameter appears in this second-order transition and every

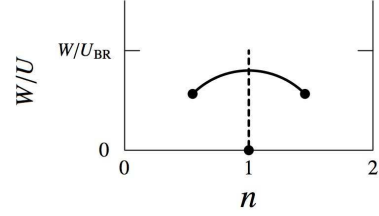


FIG. 1: Schematic phase diagram for $T = 0$ K within the subspace with no order parameter. The arc indicates a possible but unlikely first-order transition line between metallic states. Dots indicate critical points. See the text for the dashed line.

physical property seems to be continuous across the line. It is probable therefore that the critical U is infinite beyond Gutzwiller's approximation. One of the purposes of this Letter is to show that no Mott M-I transition is possible at any finite U , which contradicts a scenario that actual observed M-I transitions can be explained within the Hubbard model. Hence, the other purpose is to examine relevant effects beyond the Hubbard model, which should be considered to explain the transitions.

The Hubbard and Anderson models are defined by

$$\begin{aligned} \mathcal{H} &= \epsilon_a \sum_{i\sigma} n_{i\sigma} - \sum_{i \neq j} \sum_{\sigma} t_{ij} a_{i\sigma}^{\dagger} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1) \\ \mathcal{H}_A &= \sum_{\mathbf{k}\sigma} E_c(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma} + \frac{1}{\sqrt{N}} \sum_{\mathbf{k}\sigma} \left[V(\mathbf{k}) c_{\mathbf{k}\sigma}^{\dagger} d_{\sigma} + (\text{h.c.}) \right] \\ &\quad + \epsilon_d \sum_{\sigma} n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}. \quad (2) \end{aligned}$$

with $n_{i\sigma} = a_{i\sigma}^{\dagger} a_{i\sigma}$, $n_{d\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$, and N the number of unit cells. When it is assumed there is no order parameter, the self-energy of electrons for the Hubbard model is divided into single-site and multi-site ones: $\Sigma_{\sigma}(i\varepsilon_n, \mathbf{k}) = \tilde{\Sigma}_{\sigma}(i\varepsilon_n) + \Delta\Sigma_{\sigma}(i\varepsilon_n, \mathbf{k})$. The single-site one $\tilde{\Sigma}_{\sigma}(i\varepsilon_n)$ is given by that of the Anderson model when U and the single-site electron lines of the Feynman diagrams are the same in the two models. The chemical potentials of the

two models are denoted by μ and $\tilde{\mu}$, respectively. The single-site Green function of the Hubbard model is given by $R_\sigma(i\varepsilon_n) = (1/N) \sum_{\mathbf{k}} 1/[\varepsilon_n + \mu - E(\mathbf{k}) - \Sigma_\sigma(i\varepsilon_n, \mathbf{k})]$, with $E(\mathbf{k}) = \epsilon_a - (1/N) \sum_{i \neq j} t_{ij} \exp[i\mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)]$. Here, \mathbf{R}_i is the position of the i th lattice site. The Green function of the Anderson model is given by $\tilde{G}_\sigma(i\varepsilon_n) = 1/[i\varepsilon_n + \tilde{\mu} - \epsilon_d - \tilde{\Sigma}_\sigma(i\varepsilon_n) - L_\sigma(i\varepsilon_n)]$, with $L_\sigma(i\varepsilon_n) = (1/N) \sum_{\mathbf{k}} |V(\mathbf{k})|^2 / [i\varepsilon_n + \tilde{\mu} - E_c(\mathbf{k})]$. The condition for the electron lines is $R_\sigma(i\varepsilon_n) = \tilde{G}_\sigma(i\varepsilon_n)$. In fact, a set of $\tilde{\mu} - \epsilon_d = \mu - \epsilon_a$ and

$$L_\sigma(\varepsilon + i0) = \varepsilon + \mu - \epsilon_a - \tilde{\Sigma}_\sigma(\varepsilon + i0) - 1/R_\sigma(\varepsilon + i0), \quad (3)$$

is a mapping condition to the Anderson model. First, the multi-site self-energy is ignored in Eq. (3). The approximation is the best SSA, which considers all the single-site terms, and is reduced to a problem of determining and solving the Anderson model [8, 9, 10]. The SSA is rigorous for infinite dimensions within the Hilbert subspace with no order parameter [12]. The SSA can also be formulated as the dynamical mean-field theory (DMFT) [13, 14] and the dynamical coherent potential approximation [15].

According to Yosida's perturbation theory [16] and Wilson's renormalization-group theory [17], provided that the FS of conduction electrons is present, the ground state of the s - d model is a singlet or a normal Fermi liquid (FL). Exceptionally, it is a doublet for $J_{s-d} = 0$, with J_{s-d} the s - d exchange interaction. Since the s - d model is derived from the Anderson model, the ground state of the Anderson model is a singlet or a normal FL, or exceptionally a doublet for the just half filling and infinite U . A necessary condition for the presence of the FS is

$$\text{Im}[L_\sigma(\varepsilon + i0)]_{\varepsilon \rightarrow \pm 0} < 0. \quad (4)$$

This condition is called the FS condition in this Letter.

The density of states for $U = 0$ is given by $\rho_0(\varepsilon) = (1/N) \sum_{\mathbf{k}} \delta[\varepsilon - E(\mathbf{k})]$. It is assumed that the FS is present for $U = 0$ or that $0 < n < 2$ and there is no gap in $\rho_0(\varepsilon)$.

As a preliminary, a Lorentzian model is examined, where $\rho_0(\varepsilon)$ is given by $\rho_L(\varepsilon) \equiv (1/\pi) \Delta / [(\varepsilon - \epsilon_a)^2 + \Delta^2]$, with $\Delta > 0$. According to Eq. (3), $L_\sigma(\varepsilon + i0) = -i\Delta$ [13]. Since the FS condition (4) is satisfied for the Anderson model, the ground state of the Hubbard model is a normal FL except for $n = 1$ and $W/U = 0$.

In order to examine a non-Lorentzian model of $\rho_n(\varepsilon)$, the following model is first examined:

$$\rho_0(\varepsilon) = -\frac{1}{\pi} \text{Im} \int d\varepsilon' \frac{\rho_n(\varepsilon')}{\varepsilon - \varepsilon' + i\delta\Delta}, \quad (5)$$

with $\delta > 0$. According to Eq. (3) and the inequality $\int d\varepsilon' \rho_0(\varepsilon') [S_1(\varepsilon, \varepsilon') + x]^2 / [S_1^2(\varepsilon, \varepsilon') + S_2^2(\varepsilon)] > 0$ for any real x , with $S_1(\varepsilon, \varepsilon')$ and $S_2(\varepsilon)$ being real functions defined by $S_1(\varepsilon, \varepsilon') + iS_2(\varepsilon) = \varepsilon + \mu - \epsilon_a - \varepsilon' - \tilde{\Sigma}_\sigma(\varepsilon + i0)$, it follows that $\text{Im}L_\sigma(\varepsilon + i0) \leq 0$. The equality is only

possible provided that $\delta = +0$. The FS condition (4) is satisfied for $\delta > 0$. The ground state for $\rho_n(\varepsilon)$ is obtained in the adiabatic process $\delta \rightarrow +0$. This gives a normal FL except for $n = 1$ and $W/U = 0$, which may be degenerate with a non-normal FL provided that $\text{Im}[L_\sigma(\varepsilon + i0)]_{\varepsilon \rightarrow \pm 0, \delta \rightarrow +0} = 0$. No symmetry breaking occurs in the adiabatic process.

Since symmetry breaking is caused by Weiss mean fields, which are intersite effects, symmetry breaking is definitely impossible in the SSA, as is shown above. Under the SSA, therefore, the adiabatic continuation [18] as a function of U holds. The ground state for the non-Lorentzian $\rho_n(\varepsilon)$ is the normal FL obtained in the adiabatic process. The self-energy is expanded as $\tilde{\Sigma}_\sigma(\varepsilon + i0) = \tilde{\Sigma}_\sigma(0) + (1 - \tilde{\phi}_\gamma)\varepsilon + (1 - \tilde{\phi}_s)\frac{1}{2}\sigma g\mu_B H + O(\varepsilon^2)$ at $T = 0$ K in the presence of an infinitesimally small Zeeman energy $g\mu_B H$, with $\tilde{\Sigma}_\sigma(0)$, $\tilde{\phi}_\gamma$, and $\tilde{\phi}_s$ all being real. According to the FS sum rule [19] the electron density n is given by $n = (1/N) \sum_{\mathbf{k}\sigma} \theta([\mu - E(\mathbf{k}) - \tilde{\Sigma}_\sigma(0)]/W)$, with $\theta(x < 0) = 0$ and $\theta(x > 0) = 1$. The density of states is given by $\rho(\varepsilon) = -(1/\pi) \text{Im}R_\sigma(\varepsilon + i0)$. When n is kept constant, $\mu - \tilde{\Sigma}_\sigma(0)$, $\rho(0)$, and $L_\sigma(+i0)$ do not depend on U . Since $\text{Im}L_\sigma(+i0) < 0$ for $U = 0$, $\text{Im}L_\sigma(+i0) < 0$ for $U/W \geq 0$. When $\rho_n(\varepsilon)$ is continuous and finite, $L_\sigma(\varepsilon + i0)$ is continuous and the FS condition is satisfied so that the FL obtained in the adiabatic process is not degenerate with a non-normal FL. Provided that $\rho_n(\varepsilon)$ is discontinuous or divergent, degeneracy is possible for certain n corresponding to the discontinuity or divergence of $\rho_n(\varepsilon)$ according to the FS sum rule.

In Gutzwiller's approximation, $\tilde{\phi}_\gamma \propto 1/|1 - n|$ for $W/U = 0$. Since $\tilde{\phi}_\gamma$ diverges as $n \rightarrow 1$, $\text{Re}[\tilde{\Sigma}_\sigma(\varepsilon + i0)]_{n \rightarrow 1}$ is at least discontinuous at $\varepsilon = 0$ so that $\text{Im}[\tilde{\Sigma}_\sigma(\varepsilon + i0)]_{\varepsilon \rightarrow \pm 0, n \rightarrow 1}$ diverges logarithmically according to the Kramers-Kronig relation. Then, $\rho(\varepsilon \rightarrow \pm 0) = 0$ for $n \rightarrow 1$ and $W/U = 0$, although $\rho(0) > 0$ for $n = 1$ and $W/U \rightarrow 0$. There is a discontinuity in $\rho(\varepsilon)$ as a function of ε , n , and W/U . The critical point of $n = 1$ and $W/U = 0$ is unconventional within the SSA.

If the mapping to the Anderson model is not unique or physical quantities such as $\tilde{\phi}_\gamma$ and $\tilde{\phi}_s$ are multi-valued functions of U , a first-order transition between metallic states occurs. The adiabatic continuation still holds, for example, along a route around one of the critical points at the ends of the first-order transition line. Since the FS sum rule, $\rho(0)$, and $L_\sigma(+i0)$ are all the same in the two metallic states on different sides of the line, the occurrence of the first-order transition is unlikely. The transition never occurs in the Lorentzian model because the mapping is unique. The transition is shown on a schematic phase diagram in Fig. 1.

The occurrence of a first-order M-I transition is suggested by numerical theories using the Monte Carlo method [20] and DMFT [21]. In these theories, the compressibility $\tilde{\chi}_c(0) = dn(\mu)/d\mu$ shows a rapid change [22].

When the rapid change is really a jump, the phase diagram for $T > 0$ K is like that shown in Fig. 1 of Ref. 21. The phase diagram suggests that the first-order M-I transition occurs even at $T = 0$ K. If this is the case within the Hilbert subspace with no order parameter, however, it cannot be an M-I transition, but rather it must be a transition between metallic states.

The irreducible spin polarization function is also divided into single-site and multi-site ones: $\pi_s(i\omega_l, \mathbf{q}) = \tilde{\pi}_s(i\omega_l) + \Delta\pi_s(i\omega_l, \mathbf{q})$. The single-site one $\tilde{\pi}_s(i\omega_l)$ is given by that of the Anderson model. The spin susceptibilities of the Anderson and Hubbard models are given, respectively, by $\tilde{\chi}_s(i\omega_l) = 2\tilde{\pi}_s(i\omega_l)/[1 - U\tilde{\pi}_s(i\omega_l)]$ and $\chi_s(i\omega_l, \mathbf{q}) = 2\pi_s(i\omega_l, \mathbf{q})/[1 - U\pi_s(i\omega_l, \mathbf{q})]$. In Kondo-lattice theory, an intersite exchange interaction $I_s(i\omega_l, \mathbf{q})$ is defined by $\chi_s(i\omega_l, \mathbf{q}) = \tilde{\chi}_s(i\omega_l)/[1 - (1/4)I_s(i\omega_l, \mathbf{q})\tilde{\chi}_s(i\omega_l)]$. When $U/W \gtrsim 1$, $I_s(i\omega_l, \mathbf{q}) \simeq 2U\Delta\pi_s(i\omega_l, \mathbf{q})$, where $O[1/U\tilde{\chi}_s(i\omega_l)]$ terms are ignored. The exchange interaction is composed of three terms [23]. The first is the superexchange interaction. According to field theory, it arises from the exchange of a pair excitation of electrons between LHB and UHB. When it is assumed the widths of LHB and UHB are vanishingly small, the strength of the interaction between nearest neighbors is $J = -4|t|^2/U$, with t the transfer integral between nearest neighbors [24]. The second is an exchange interaction arising from the exchange of a pair excitation of the quasiparticles. The strength of the interaction is proportional to the bandwidth of the quasiparticles. It is antiferromagnetic when the nesting of the FS is sharp or the chemical potential lies around the band center of the quasiparticles, and it is ferromagnetic when the chemical potential lies around one of the band edges of the quasiparticles. The third term corresponds to the mode-mode coupling term in the self-consistent renormalization theory of spin fluctuations [25], which is relevant for $U/W \lesssim 1$. According to the Ward relation [26], the static component of the single-site irreducible vertex function in spin channels is given by $\tilde{\lambda}_s = \tilde{\phi}_s[1 - U\tilde{\pi}_s(0)]$. When this is used, the mutual interaction between the quasiparticles is given by $(U\tilde{\lambda}_s)^2[\chi_s(i\omega_l, \mathbf{q}) - \tilde{\chi}_s(i\omega_l)] = \tilde{\phi}_s^2 I_s^*(i\omega_l, \mathbf{q})$, with $I_s^*(i\omega_l, \mathbf{q}) = I_s(i\omega_l, \mathbf{q})/[1 - (1/4)I_s(i\omega_l, \mathbf{q})\tilde{\chi}_s(i\omega_l)]$; the single-site term is subtracted because it is considered in the SSA. The mutual interaction mediated by spin fluctuations is essentially the same as that due to the exchange interaction $I_s(i\omega_l, \mathbf{q})$ or $I_s^*(i\omega_l, \mathbf{q})$. In Kondo-lattice theory, an unperturbed state is constructed in the non-perturbative SSA theory [27] and intersite effects are perturbatively considered in terms of $I_s(i\omega_l, \mathbf{q})$ [28].

When the Fock-type self-energy due to the superexchange interaction J is considered, the bandwidth of the quasiparticles is given by $W^* \propto (W/\tilde{\phi}_\gamma) + c_J|J|$, with $c_J = O(1)$ [29]. When this renormalization is considered, the critical point of $n = 1$ and $W/U = 0$ turns conventional; there is no discontinuity in $\rho(\varepsilon)$ as a function of ε , n , and W/U .

An order parameter can appear in two dimensions or higher. The stability of a normal FL against an ordered state with an order parameter can be examined when the corresponding response function is perturbatively considered in terms of $I_s(i\omega_l, \mathbf{q})$ or $I_s^*(i\omega_l, \mathbf{q})$. When $I_s(i\omega_l, \mathbf{q})$ is strong, for example, the FL is unstable against a magnetic state. The Néel temperature T_N is defined as the highest value of T_N determined by $[\chi_s(0, \mathbf{q})]_{T=T_N} \rightarrow +\infty$ as a function of \mathbf{q} . When $I_s(i\omega_l, \mathbf{q})$ is so weak that $[\chi_s(0, \mathbf{q})]_{T=0\text{K}} < +\infty$ for any \mathbf{q} , the FL is stable against any magnetic state.

The energy scale of local quantum spin fluctuations is defined by $k_B T_K = 1/[\tilde{\chi}_s(0)]_{T=0\text{K}}$, where T_K is the so-called Kondo temperature. In accordance with the T -dependent crossover between a localized spin for $T \gg T_K$ and a normal FL for $T \ll T_K$ in the Kondo problem [17], magnetism for $T_N \gg T_K$ is characterized as local-moment magnetism and magnetism for $T_N \ll T_K$ is characterized as itinerant-electron magnetism [29]. The magnetism crossover is simply a Mott M-I crossover.

When $I_s^*(i\omega_l, \mathbf{q})$ is weak or strong, the FL is unstable against an anisotropic superconducting (SC) state at least at $T = 0$ K, provided that no disorder exists. When $I_s^*(i\omega_l, \mathbf{q})$ is antiferromagnetic, the FL is unstable against a singlet SC state. For example, it has been proposed [30, 31] that the condensation of $d\gamma$ -wave Cooper pairs of the Gutzwiller quasiparticles due to the superexchange interaction is responsible for high- T_c superconductivity [32], which occurs in the vicinity of the Mott M-I crossover. When $I_s^*(i\omega_l, \mathbf{q})$ is ferromagnetic, the FL is unstable against a triplet SC state.

The FL can also be unstable against a bond-order (BO) state, whose order parameter is $\langle a_{i\sigma}^\dagger a_{j\sigma'} \rangle_{i \neq j}$, and a flux state, which is a superposition of several BO states. Within Kondo-lattice theory, magnetic or SC states are more stable than BO and flux states.

When $U/W \lesssim 1$, the conventional perturbation in terms of U is more useful than that in terms of $I_s(i\omega_l, \mathbf{q})$. A similar argument to that for $U/W \gtrsim 1$ applies in this case. When the nesting of the FS is sharp, a non-interacting electron gas is unstable against a spin density wave. When an interaction between electrons given by $U^2\chi_s(i\omega_l, \mathbf{q})$ is considered, the electron gas is unstable against an anisotropic SC state at least at $T = 0$ K, provided that no disorder exists.

No order parameter appears in one dimension. The FL for $U/W \gtrsim 1$ becomes a Tomonaga-Luttinger liquid when $I_s(i\omega_l, \mathbf{q})$ is perturbatively treated, as the electron gas does when U is perturbatively treated. It is probable that Lieb and Wu's insulating state for the just half filling [33] can only be obtained by non-perturbative theory.

In this analysis, the ground state is not a paramagnetic Mott insulator except for $n = 1$ and $W/U = 0$. However, since the nature of actual M-I transitions cannot be explained within the Hubbard model, various effects should be considered in a multi-band or multi-orbital

model. Changes of lattice symmetries or jumps in lattice constants are often observed [2], which implies that the electron-phonon interaction should also be considered. A relevant electron-phonon interaction must arise from spin and orbital channels [34]. Cooperative Jahn-Teller or orbital ordering must be responsible for the change of lattice symmetries. As well as the electron-phonon interaction, the orbital-channel exchange interaction can play a role in the ordering.

The FS sum rule holds for the Gutzwiller quasiparticles. The ordinary rule holds in the absence of an order parameter, and a modified rule holds even when the Brillouin zone is folded by an antiferromagnetic or orbital order parameter. Then, Wilson's classification of crystalline solids into metals and insulators [35] can apply to M-I transitions. Two types of M-I transitions are possible according to the band structures of the quasiparticles in the absence and presence of an order parameter: between a metal and an insulator and between a compensated metal and an insulator. The Kondo temperature T_K can be different in metallic and insulating phases of a first-order M-I transition. In the metallic phase, T_K is higher than T and the quasiparticles are well defined. If T_K is lower than T in the insulating phase, the quasiparticles are not well defined. In such a case, the M-I transition is a transition between a high- T_K itinerant-electron phase and a low- T_K local-moment phase. Change of lattice symmetries or jumps in lattice constants must play a crucial role in any first-order M-I transition.

Since disorder, either small or large, must always exist, Anderson localization and other effects due to disorder [29] can play a role in actual M-I transitions or crossovers.

In conclusion, the ground state of the Hubbard model is not a paramagnetic Mott insulator except for $n = 1$ and $W/U = 0$ in two and higher dimensions. In order to explain actual M-I transitions, the electron-phonon interaction, multi-band or multi-orbital effects, and the effects of disorder should be considered beyond the Hubbard model. Except for the low- T_K local-moment phase of electrons, whether a crystalline solid is a metal or an insulator can be explained by an extended Wilson's classification of the band structure of quasiparticles in the absence or presence of an order parameter.

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